Spin and orbital moments in Fe and Co systems with various dimensionalities

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Collaborators

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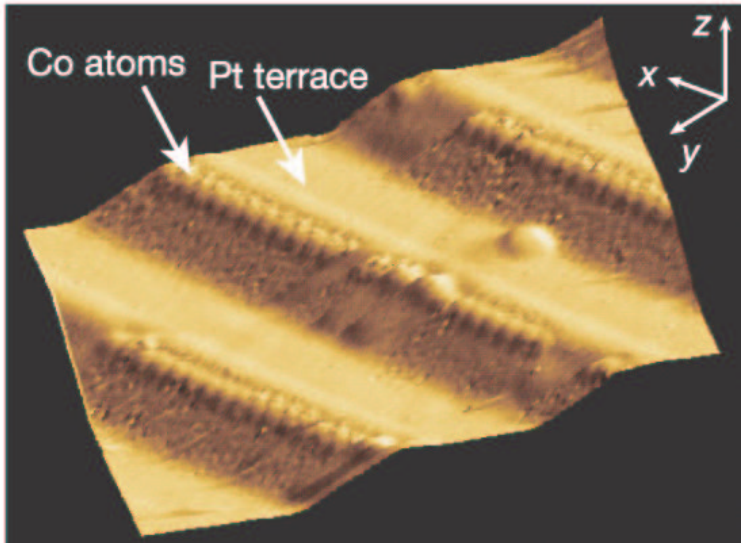
Low-dimensional magnetic systems

Gambardella et al., Nature 416, 301 (2002): "Ferromagnetism in one-dimensional monatomic metal chains"



- monatomic Co chains on a vicinal Pt surface
- magnetic measurements using XMCD
- blocking temperature $T_{\mathrm{B}} \approx 15K$
- orbital moment: 0.68 μ_{B}
- very large anisotropy energy (50 x bulk)

$\Rightarrow$ Predictive capabilities for magnetic moments and anisotropy energy in low-dimensional magnetic systems?

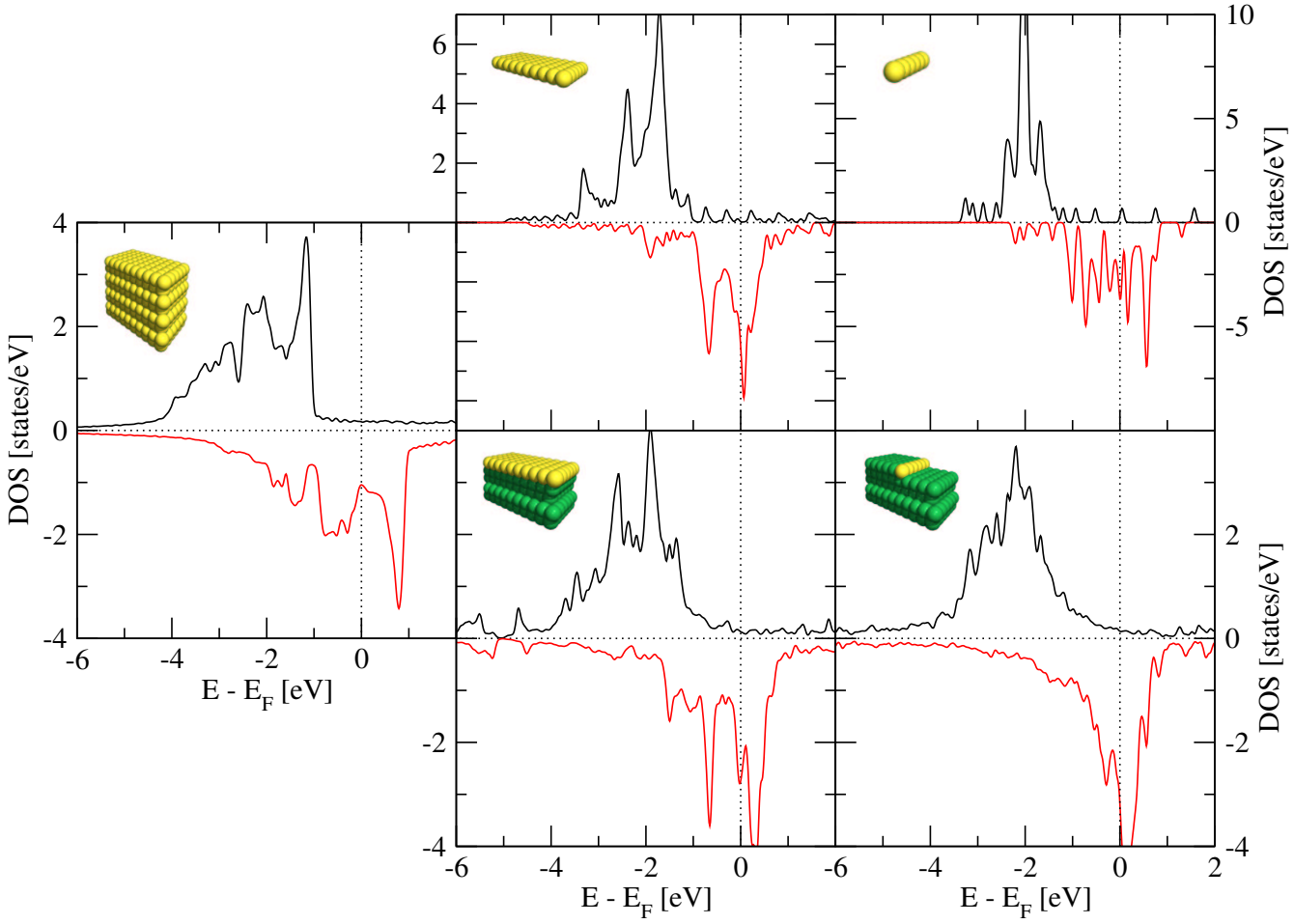
Investigated Systems

- 3D, 2D, and 1D systems (Fe and Co) with and without Pt substrate

- no structural relaxation, close-packed parent lattice with exp. Pt lattice constant
- LMTO-ASA with spin-orbit coupling (SOC), cross-checked with FLAPW
- pure LSDA, LSDA+OP, LSDA+U (always with SOC!)

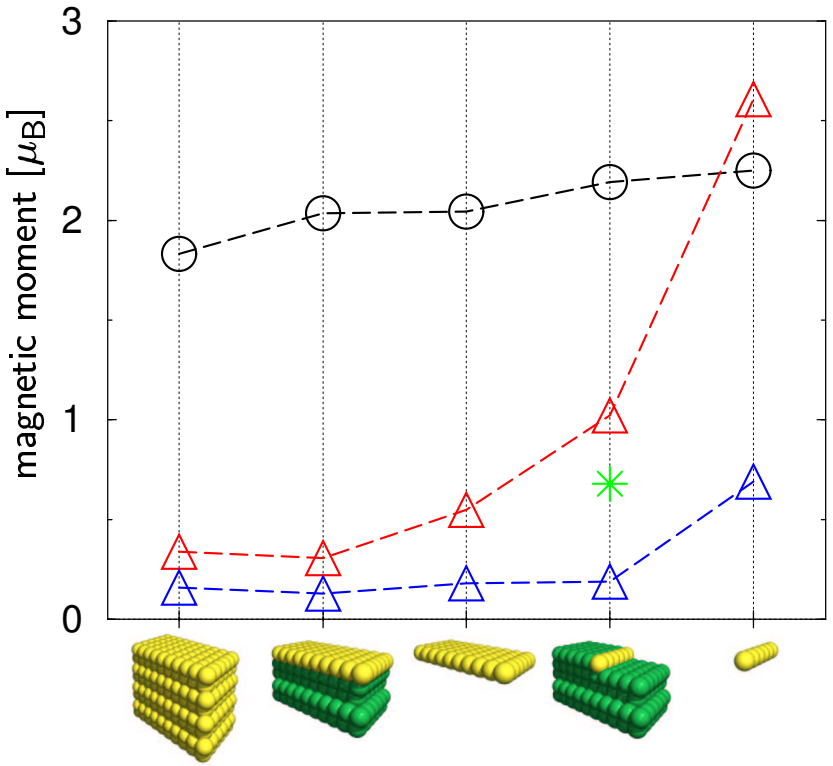
Strongly correlated systems?

Reduction of dimensionality leads to band-narrowing.

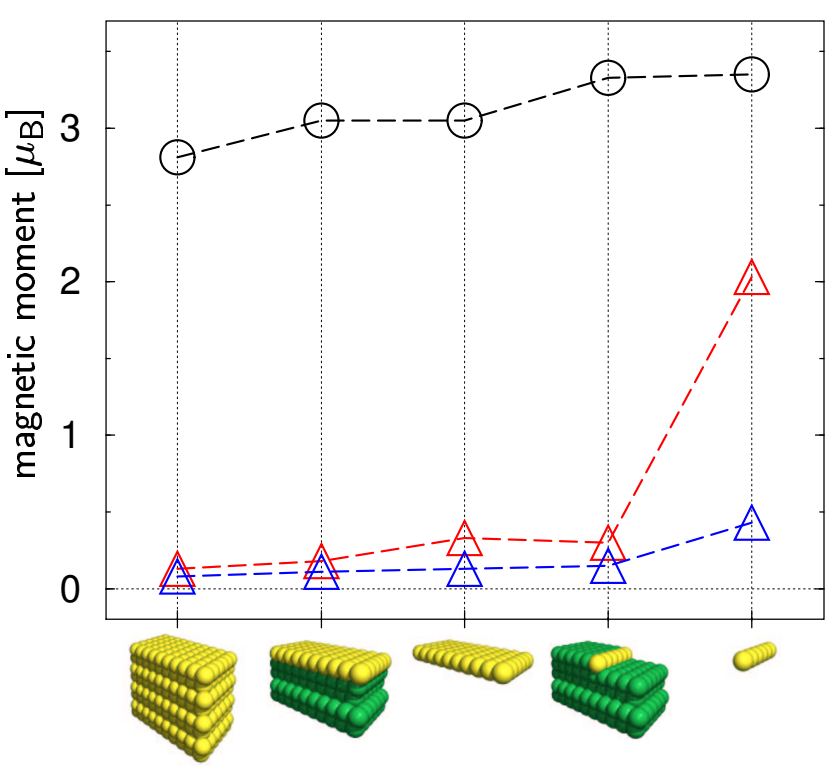


Spin and orbital moments in systems with various dimensionalities

Co:



Fe:



⊖–⊖ spin moment
△–△ orbital moment (LSDA+OP)
△–△ orbital moment (LSDA)
✳ Exp. (Gambardella et al.)

- pure LSDA is not able to describe strong increase of orbital moment
- orbital moment is substantially reduced by substrate

A little bit of theory

pure LSDA: just spin-orbit coupling

LSDA+OP: Eriksson et al., Phys. Rev. B 42, 2707 (1990)

$$E = E_{\text{LSDA}} - \frac{1}{2} B \langle L_z \rangle^2$$

Racah Parameter: $B = \frac{1}{441}(9F^2 - 5F^4)$

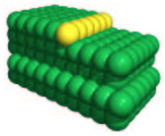
Solovyev et al., Phys. Rev. Lett. 80, 5758 (1998): LSDA+OP is included in LSDA+U

$$E = E_{\text{LSDA}} + E_{\text{ee}} - E_{\text{dc}}$$

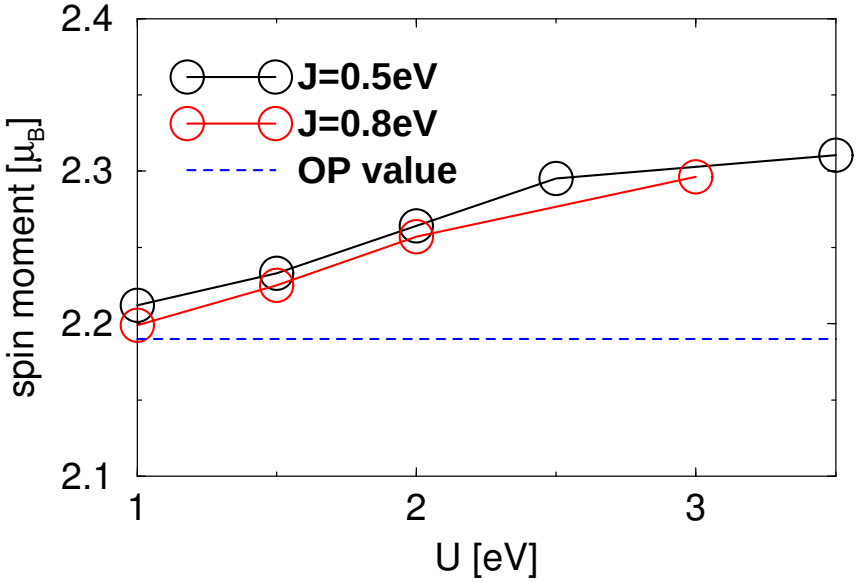
$$E_{\text{ee}} = \frac{1}{2} \sum_{\{\gamma\}} \left(U_{\gamma_1\gamma_3\gamma_2\gamma_4} - U_{\gamma_1\gamma_3\gamma_4\gamma_2} \right) n_{\gamma_1\gamma_2} n_{\gamma_3\gamma_4} \quad , \quad \gamma = (s, m)$$

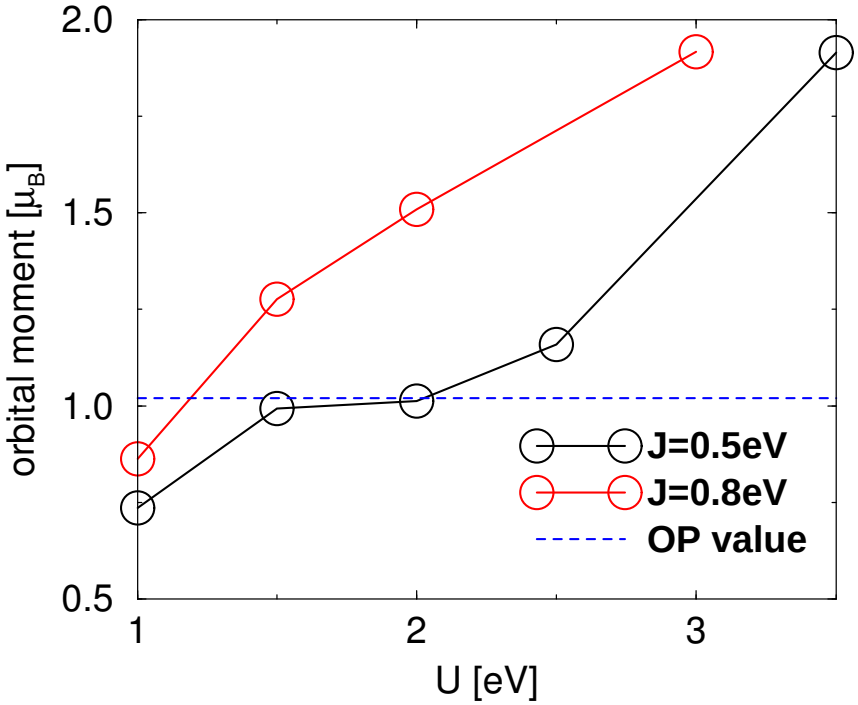
$$E_{\text{dc}} = \frac{U}{2} n(n+1) - \frac{J}{2} \sum_s n_s(n_s + 1)$$

LSDA+U results



Calculations for a Co wire
on a vicinal Pt surface.





$\rightarrow$ Similar values as with LSDA+OP for $U = 1 \ldots 2eV$, $J = 0.5 \ldots 0.8eV$

Conclusions and open questions

- Correlation effects become more important in low-dimensional systems.
- LSDA+OP seems to give reasonable results for the orbital moments but is not very satisfying from a theoretical point of view.
- LSDA+U also gives results comparable to LSDA+OP, but are the values for U and J reasonable?

$\rightarrow$ There is no *safe* method for calculating orbital moments (and anisotropy!) in low-dimensional systems.